CENTRAL UNIVERSITY OF KERALA
DEPARTMENT OF CHEMISTRY
M.Sc. CHEMISTRY

Course Code	Course Title	Contact hrs. / wk.				Credits
		Lect.	Lab	Tut	Total	
CHE 5003	Computational Chemistry	2	1	1		3

Lec = Lecture, Tut = Tutorial, Lab = Practical

This is a participatory, experimental, and employability based skill development course.

Course objective:

This course is aimed to train students to solve chemistry problems by using computing tools and to apply this knowledge in interdisciplinary areas of science.

By completing this course, students will obtain the following course/learning outcomes:

- Understanding of the basic principles of computational chemistry.
- Performance of simple computational experiments such as energy evaluation, transition state modeling, conformational analysis.
- Skill development to design, perform and analyze chemistry problems using computational tools.

Grading:

Computational Lab Experiments – 15%
Assignments and / seminar – 10%
Internal assessment tests – 15%
End Semester Assessment – 60%

CHE 5003   Computational Chemistry

Syllabus Modules:

- Molecular Mechanics. Potential energy surfaces. Curve crossing Model. Force field.
- Factors governing barrier heights. Quantum Mechanical and Molecular Mechanics potential functions.
- MM force fields. Parametrization. Steric energies, Heats of formation and strain.
- Computational chemistry lab: Z-matrix specification, Input for Semi-empirical and *ab-initio* programs. Molecular mechanics program. Analysis of output.

References

1.   F. Jensen, Introduction to computational chemistry, Wiley, NY, 2007.

2.   D. C. Young, Computational Chemistry, John-Wiley and Sons, NY, 2001.

3.   C. J. Cramer, Essentials of Computational Chemistry, John-Wiley & Sons, 2004.

4.   U. Burkert and N.L. Allinger: Molecular Mechanics, ACS Monograph, American Chemical   Society, 1977.

5.   Albright, Burdett and Whanghbo, Approximate Molecular Orbital Theory, Academic Press, 1985.

6.   MOPAC 6.0 Manual and computer program, QCPE Ed.

7.   PCMODEL Manual and Computer program, Serena Software.